Vacuum-polarization screening corrections to the energy levels of lithiumlike ions

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Calculations of the vacuum-polarization corrections to the low-lying energy levels of Li-like highly charged ions are presented. The calculations are carried out for extended nuclei in the range $Z=20-100$. [S1050-2947(99)01406-7]

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INTRODUCTION

Currently, enormous progress is achieved both in experimental and theoretical investigations on heavy highly charged ions. These investigations are extremely important as they provide the unique possibility to examine quantum electrodynamics (QED) in extremely strong electric fields.

In particular, an outstanding experimental precision was reached in Lamb shift measurements of lithiumlike ions. Schweppe *et al.* reported a value of 280.59 ± 0.09 eV for the $(1s)^2 2p_{1/2}\rightarrow(1s)^2 2s$ transition energy in U^{89+} [1]. The energy difference between the $(1s)^2 2p_{3/2}$ and the $(1s)^2 2s$ states was measured with even higher accuracy for Li-like Bi, where 2788.14 ± 0.04 eV was obtained [2]. Recently, this series was continued by very precise measurements in Li-like Ni, Zn, and Ag [3,4]. It is expected that the accuracy for Li-like heavy ions as gold, lead, bismuth, and uranium, will even increase in the near future due to experimental techniques currently under development at GSI [5].

This experimental precision challenges theoreticians to perform calculations, which meet at least the same level of accuracy. This aim requires, in particular, to take into account quantum electrodynamical (QED) corrections of second order in α. The one-electron QED corrections of this order were partially calculated in [6–16] and a recent review was published by Mohr *et al.* [17]. However, since the complete gauge invariant set of the self-energy–self-energy diagrams has not yet been calculated [15,16,18,19], the total value of the one-electron QED correction of second order in α remains yet unknown. Concerning the two-electron QED corrections precise calculations up to the second-order in α were carried out only for the ground state of He-like ions [20–24]. Evaluations of the second-order two-electron corrections in Li-like ions were performed by several authors using approximative approaches [25–28]. A complete accurate calculation was presented recently for the self-energy screening diagrams in the case of the $(1s)^2 2s$ state in the range $Z=20-100$ [29]. In [30], the self-energy screening diagrams and the vacuum-polarization screening diagrams were calculated for the $(1s)^2 2s$ and $(1s)^2 2p_{1/2}$ states for $Z=83$ and $Z=92$. The major aim of this paper is to perform a complete evaluation of the vacuum polarization screening contribution in a wide interval of Z. We consider corrections to the $(1s)^2 2s$ state, to the $(1s)^2 2p_{1/2}$ state, and to the $(1s)^2 2p_{3/2}$ state of Li-like ions.

First, we derive the basic formulas. Then we describe details of our numerical calculations and present the results which are compared to approximative results of former calculations. Throughout the paper, we use relativistic units ($\hbar=c=m_e=1$).

I. BASIC FORMULAS

The Feynman diagrams for the vacuum-polarization corrections are shown in Fig. 1. For the case of a Li-like ion with a closed $(1s)^2$ shell plus an additional electron, it is possible to divide the vacuum-polarization screeening diagrams into two subsets: one corresponding to the interaction between two electrons of the closed $(1s)^2$ shell (δE^{1s}_{1s}) and the other corresponding to the interaction between the closed $1s$ shell and the valence electron ($\delta E^{v}_{(1s)^2}$). Calculations of δE^{1s}_{1s} were already performed in [23]. Therefore, we will concentrate in this paper on the calculation of the second subset of the diagrams.

The formal expressions for the diagrams shown in Fig. 1 can be easily derived using the two-time Green's function method [31]. It is convenient to divide the contribution of the diagrams shown in Fig. 1(a) into two pieces: an *irreducible* one and a *reducible* one. In the irreducible part, the energy of the intermediate electron state is not equal to that of the initial state. The reducible part is formed by the remainder.

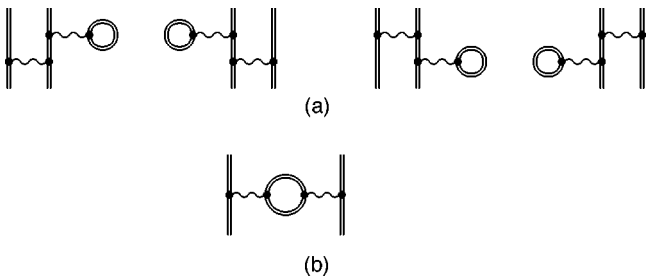

FIG. 1. Vacuum polarization screening diagrams.

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For the diagrams shown in Fig. 1(a), the irreducible contribution is given by

$$\Delta E_a^{\rm irred}=2\sum_{m_a}\{\langle a|U_{VP}^a|\xi_a\rangle+\langle b|U_{VP}^a|\xi_b\rangle\}, \tag{1}$$

$$|\xi_a\rangle=\sum_{\varepsilon_n\neq\varepsilon_a}\frac{|n\rangle}{\varepsilon_a-\varepsilon_n}\{\langle nb|I(0)|ab\rangle-\langle bn|I(\delta)|ab\rangle\}, \tag{2}$$

$$|\xi_b\rangle=\sum_{\varepsilon_n\neq\varepsilon_b}\frac{|n\rangle}{\varepsilon_b-\varepsilon_n}\{\langle na|I(0)|ba\rangle-\langle an|I(\delta)|ba\rangle\}. \tag{3}$$

Here $U_{\rm VP}^a$ is the vacuum polarization potential,

$$U_{\rm VP}^a(\mathbf{x})=\frac{\alpha}{2\pi i}\int d\mathbf{y}\frac{1}{|\mathbf{x}-\mathbf{y}|}\int_{-\infty}^{\infty}d\omega\,{\rm Tr}[G(\omega,\mathbf{y},\mathbf{y})], \tag{4}$$

$$I(\omega,|\mathbf{x}-\mathbf{y}|)=\alpha\frac{\alpha_{1\mu}\alpha_2^{\mu}}{|\mathbf{x}-\mathbf{y}|}\exp(i|\omega||\mathbf{x}-\mathbf{y}|), \tag{5}$$

$\alpha^{\mu}\equiv(1,\boldsymbol{\alpha})$, $\boldsymbol{\alpha}$ are the Dirac matrices; a is the $1s$ state with a spin projection m_a, b is the valence state, $G(\omega,\mathbf{x},\mathbf{y})=\Sigma_n\psi(\mathbf{x})\psi^{\dagger}(\mathbf{y})/[\omega-\varepsilon_n(1-i0)]$ is the Coulomb Green function, and $\delta=\varepsilon_b-\varepsilon_a$.

For the reducible part one obtains

$$\Delta E_a^{\rm red}=-\sum_{m_a}\langle ba|I'(\delta)|ab\rangle\{\langle b|U_{VP}^a|b\rangle-\langle a|U_{VP}^a|a\rangle\}, \tag{6}$$

where $I'(\delta)=(d/d\omega)I(\omega)|_{\omega=\delta}$.

The contribution of the diagrams shown in Fig. 1(b) is given by

$$\Delta E_b=\sum_{m_a}\{\langle ab|U_{VP}^b(0)|ab\rangle-\langle ba|U_{VP}^b(\delta)|ab\rangle\}, \tag{7}$$

where

$$U_{VP}^b(\varepsilon,\mathbf{x},\mathbf{y})=\frac{\alpha^2}{2\pi i}\int_{-\infty}^{\infty}d\omega\int d\mathbf{z}_1\int d\mathbf{z}_2\frac{\alpha_{1\mu}\exp(i|\varepsilon||\mathbf{x}-\mathbf{z}_1|)}{|\mathbf{x}-\mathbf{z}_1|}\frac{\alpha_{2\nu}\exp(i|\varepsilon||\mathbf{y}-\mathbf{z}_2|)}{|\mathbf{y}-\mathbf{z}_2|}{\rm Tr}\left[\alpha^{\mu}G\left(\omega-\frac{\varepsilon}{2},\mathbf{z}_1,\mathbf{z}_2\right)\alpha^{\nu}\times G\left(\omega+\frac{\varepsilon}{2},\mathbf{z}_2,\mathbf{z}_1\right)\right]. \tag{8}$$

The contributions (1), (6), and (7) are ultraviolet divergent. The renormalization of these contributions is performed in the same way as in [23]. In contrast to the ground-state calculations of He-like ions [23], the energy variables of the Green's functions in Eq. (8) do not coincide for the exchange term. Therefore, a reanalysis of the spurious gauge-dependent piece of the light-by-light scattering contribution is required. It was shown before [23,32–34], that no spurious contribution exists in the case of one-electron vacuum-polarization corrections and vacuum-polarization screening corrections to the ground-state energy of He-like ions, if these calculations are based on the partial wave expansion of the electron Green's function and the sum over the angular momentum quantum number κ is restricted to a finite number of terms ($|\kappa|\leqslant K$). We found that this rule remains to be valid also in the case of the diagrams shown in Fig. 1(b) if the energies of the Green's functions do not coincide. A proof is presented in the Appendix.

II. CALCULATION

The calculation of Eq. (1) was performed in the same way as in [23]. The formulas for the Uehling and the Wichmann-Kroll potentials are well known:

$$U_{\rm Uehl}^a(r)=-\alpha Z\frac{2\alpha}{3\pi}\int_0^{\infty}dr'\,4\pi r'\rho(r')\int_1^{\infty}dt\left(1+\frac{1}{2t^2}\right)\frac{\sqrt{t^2-1}}{t^2}\frac{\{\exp(-2m|r-r'|t)-\exp[-2m(r+r')t]\}}{4mrt}, \tag{9}$$

$$U_{\rm WK}^a(x)=\frac{2\alpha}{\pi}\sum_{\kappa=\pm1}^{\pm\infty}|\kappa|\int_0^{\infty}d\omega\int_0^{\infty}dy\,y^2\int_0^{\infty}dz\,z^2\frac{1}{\max(z,y)}V(z)\sum_{i,k=1}^{2}{\rm Re}\{F_{\kappa}^{ik}(i\omega,y,z)[G_{\kappa}^{ik}(i\omega,y,z)-F_{\kappa}^{ik}(i\omega,y,z)]\}, \tag{10}$$

where G_{κ}^{ik} and F_{κ}^{ik} are the radial components of the partial-wave contributions to the bound and free electron Green's functions, respectively.

For the Uehling contribution, a Fermi-like nuclear charge distribution was assumed. The wave function and the reducible Green's function for this charge distribution were obtained using the *B*-spline method for solving the Dirac equation [35]. The remaining Wichmann-Kroll-potential charge density was calculated for a nuclear charge distribution equal to a homogeneously charged spherical shell. For this model,

TABLE I. The vacuum-polarization correction due to the interaction of the valence electron with the closed $(1s)^2$ shell. Energy values are given in eV.

Z	$\langle r^2\rangle^{1/2}$ (fm)	$\delta E^{2s}_{(1s)^2}$	$\delta E^{2p_{1/2}}_{(1s)^2}$	$\delta E^{2p_{3/2}}_{(1s)^2}$	$\delta E^{2p_{1/2}}_{(1s)^2}-\delta E^{2s}_{(1s)^2}$	$\delta E^{2p_{3/2}}_{(1s)^2}-\delta E^{2s}_{(1s)^2}$
20	3.478	0.0032	0.0009	0.0008	−0.0023	−0.0024
28	3.769	0.0088	0.0025	0.0022	−0.0063	−0.0067
30	3.928	0.0109	0.0031	0.0027	−0.0078	−0.0083
32	4.072	0.013	0.0039	0.0032	−0.0096	−0.0102
40	4.270	0.0277	0.0084	0.0064	−0.0193	−0.0213
47	4.542	0.0481	0.0156	0.0106	−0.0325	−0.0374
50	4.655	0.0599	0.0200	0.0129	−0.0399	−0.0470
54	4.787	0.0793	0.0276	0.0165	−0.0518	−0.0628
60	4.914	0.1188	0.0441	0.0233	−0.0746	−0.0954
66	5.224	0.1749	0.0699	0.0321	−0.1050	−0.1428
70	5.317	0.2249	0.0948	0.0392	−0.1301	−0.1856
74	5.373	0.2886(1)	0.1286	0.0476	−0.1600(1)	−0.2409(1)
79	5.437	0.3932(1)	0.1884	0.0602	−0.2049(1)	−0.3330(1)
80	5.467	0.4182(1)	0.2034(1)	0.0629	−0.2149(1)	−0.3553(1)
82	5.505	0.4732(3)	0.2372(1)	0.0689	−0.2360(3)	−0.4043(3)
83	5.533	0.5034(3)	0.2564(1)	0.0719	−0.2471(3)	−0.4314(3)
90	5.802	0.7775(4)	0.4443(2)	0.0973	−0.3332(4)	−0.6803(4)
92	5.860	0.8815(5)	0.5216(3)	0.1056(1)	−0.3598(6)	−0.7760(5)
100	5.886	1.475(1)	1.0144(8)	0.1460(1)	−0.460(1)	−1.329(1)

exact solutions for the radial components of the Green's function can be employed [34]. The same scheme was employed to calculate the vacuum-polarization potential in Eq. (6).

The contribution of the diagrams shown in Fig. 1(b) was also divided into two parts: the leading (Uehling) contribution and the remaining (Wichmann-Kroll) term. The expression for the Uehling contribution can be obtained by replacing the usual photon propagator $D_{\mu\nu}$ by an ''effective'' photon propagator,

$$\tilde{D}_{\mu\nu}(k^2)=\frac{\alpha}{\pi}D_{\mu\nu}(k^2)(-k^2)\int_0^1 dv\,\frac{v^2(1-\frac{1}{3}v^2)}{4m^2-k^2(1-v^2)-i0}, \tag{11}$$

where $k^2=\varepsilon^2-\mathbf{k}^2$ (see, e.g., [36]). Utilizing Eq. (11) one obtains the following expression for the Uehling operator:

$$U^b_{\rm Uehl}(\varepsilon,\mathbf{x},\mathbf{y})=\alpha\frac{\alpha_{1\mu}\alpha_2^{\mu}}{|\mathbf{x}-\mathbf{y}|}\frac{2\alpha}{3\pi}\int_1^{\infty}dt\left(1+\frac{1}{2t^2}\right)\frac{\sqrt{t^2-1}}{t^2}$$
$$\times\exp(-\sqrt{(2mt)^2-\varepsilon^2}|\mathbf{x}-\mathbf{y}|), \tag{12}$$

where ε is the energy of the transmitted photon.

The Wichmann-Kroll contribution to the diagram (b) in Fig. 1 was calculated utilizing the partial differences between the expression (8) and the corresponding equation with the bound-electron Green's functions replaced by those of free electrons. In this calculation some large terms appear, which almost cancel each other. To improve the numerical cancelation of these terms we employed a procedure similar to the one in [23]. This Wichmann-Kroll part was calculated only for the point-nucleus case. Finite-size effects can be neglected due to its smallness compared to the other contributions.

The numerical results of our calculation are presented in Table I. The values of the root-mean-square charge radii were taken from [37,38].[1] To obtain a reasonable estimate for the precision of our values, the indicated root-mean-square charge radii were changed by one percent. The difference between both results yields the indicated uncertainty. In Table II we present the different contributions of the vacuum-polarization correction to the energy levels of Li-like uranium in detail.

It is illuminating to compare our results with the previous calculations of these corrections. For the $(1s)^2 2p_{1/2}\rightarrow(1s)^2 2s$ transition in Li-like uranium we obtain $-0.3598(6)$ eV. This result is in reasonable agreement with the previous results which read $-0.39(1)$ [27], -0.39 [28], and -0.41 [26].

[1]For $Z=90$ we also recalculate δE^{1s}_{1s} with $\langle r^2\rangle^{1/2}=5.802$ fm [38] (in [23] $\langle r^2\rangle^{1/2}=5.645$ fm was used). Using this value of the root-mean-square radius gives $\delta E^{1s}_{1s}=2.338(1)$ eV instead of $\delta E^{1s}_{1s}=2.341(1)$ [23].

TABLE II. Various components of the vacuum-polarization correction in Li-like uranium. Values are given in eV.

Contribution	$(1s)^2 2s$	$(1s)^2 2p_{1/2}$	$(1s)^2 2p_{3/2}$
$\delta E^{a,\rm irred}_{Ue}$	0.8961(5)	0.5374(3)	0.1300(1)
$\delta E^{a,\rm red}_{\rm Uehl}$	−0.0085	−0.0146	−0.0235
δE^{b}_{Ue}	0.0382	0.0313	0.0059
$\delta E^{a,\rm irr}_{\rm WK}$	−0.0426	−0.0319	−0.0079
$\delta E^{a,\rm red}_{\rm WK}$	0.0005	0.0008	0.0012
$\delta E^{b}_{\rm WK}$	−0.0021	−0.0013	−0.0002
Total contribution	0.8815(5)	0.5216(3)	0.1056(1)

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APPENDIX

It is convenient to divide the light-by-light scattering contribution of the diagram shown in Fig. 1(b) into two parts, one corresponding to the direct diagram and the other corresponding to the exchange diagram. The direct part can be handled in the same way as in [23]. So, we restrict our consideration to the exchange part, which is given by

$$\Delta E = -e^4 \xi, \tag{A1}$$

$$\begin{aligned}\xi = \frac{i}{2\pi} \sum_{m_{1s}} \int_{C_F} d\omega \int d\mathbf{x}_1\, d\mathbf{x}_2\, A_\mu^{(a)}(\mathbf{x}_1) A_\nu^{(b)}(\mathbf{x}_2) \int d\mathbf{y}_1\, d\mathbf{y}_2\, \mathrm{Tr}[\, \alpha^\mu F(\omega+\delta,\mathbf{x}_1,\mathbf{y}_1) V(\mathbf{y}_1) F(\omega+\delta,\mathbf{y}_1,\mathbf{x}_2) \\ \times \alpha^\nu F(\omega,\mathbf{x}_2,\mathbf{y}_2) V(\mathbf{y}_2) F(\omega,\mathbf{y}_2,\mathbf{x}_1) + \alpha^\mu F(\omega+\delta,\mathbf{x}_1,\mathbf{x}_2) \alpha^\nu F(\omega,\mathbf{x}_2,\mathbf{y}_1) V(\mathbf{y}_1) F(\omega,\mathbf{y}_1,\mathbf{y}_2) V(\mathbf{y}_2) F(\omega,\mathbf{y}_2,\mathbf{x}_1) \\ + \alpha^\mu F(\omega+\delta,\mathbf{x}_1,\mathbf{y}_1) V(\mathbf{y}_1) F(\omega+\delta,\mathbf{y}_1,\mathbf{y}_2) V(\mathbf{y}_2) F(\omega+\delta,\mathbf{y}_2,\mathbf{x}_2) \alpha^\nu F(\omega,\mathbf{x}_2,\mathbf{x}_1)\,],\end{aligned} \tag{A2}$$

where $A_\mu^{(a)}(\mathbf{x}) = \int d\mathbf{y}\, \psi_{1s}^\dagger(\mathbf{y}) \alpha^\nu D_{\nu\mu}(\delta,\mathbf{x}-\mathbf{y}) \psi_{2n}(\mathbf{y})$, $A_\mu^{(b)}(\mathbf{x}) = \int d\mathbf{y}\, \psi_{2n}^\dagger(\mathbf{y}) \alpha^\nu D_{\nu\mu}(\delta,\mathbf{x}-\mathbf{y}) \psi_{1s}(\mathbf{y})$, m_{1s} is the spin projection of $1s$ state, $D_{\nu\mu}(\omega,\mathbf{x}-\mathbf{y})$ is the photon propagator, $F(\omega,\mathbf{x},\mathbf{y})$ is the free-electron propagator, δ is the energy difference between the valence electron and the $1s$ electron.

If we write $F(\omega+\delta,\mathbf{x},\mathbf{y})$ as

$$F(\omega+\delta,\mathbf{x},\mathbf{y}) = F(\omega,\mathbf{x},\mathbf{y}) + [F(\omega+\delta,\mathbf{x},\mathbf{y}) - F(\omega,\mathbf{x},\mathbf{y})], \tag{A3}$$

the total contribution (A2) can be divided into two parts:

$$\xi = \xi^0 + \xi^\delta, \tag{A4}$$

where ξ^0 contains only $F(\omega)$ and ξ^δ contains various combinations of $F(\omega)$ and $[F(\omega+\delta) - F(\omega)]$. The evaluation of ξ^0 is similar to that outlined in [23]. So, we restrict our consideration to the term ξ^δ.

Let us write $[F(\omega+\delta,\mathbf{x},\mathbf{y}) - F(\omega,\mathbf{x},\mathbf{y})]$ as

$$F(\omega+\delta,\mathbf{x},\mathbf{y}) - F(\omega,\mathbf{x},\mathbf{y}) = \sum_{n=1}^{\infty} (-1)^n \delta^n \int dz_1 \ldots \int dz_n\, F(\omega,\mathbf{x},\mathbf{z}_1) \ldots F(\omega,\mathbf{z}_n,\mathbf{y}). \tag{A5}$$

From this, it is clear that the term ξ^δ can be handled in the same way as the diagrams containing five and more vertices on the vacuum loop. It is well known that these diagrams do not contain spurious gauge-dependent pieces. Hence, the whole contribution (A1) does not contain any spurious gauge-dependent terms if we use the calculation scheme based on the partial wave expansion of the electron Green function.

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